estimate of the power required to establish a self-trapped filament of less than 10 μm diameter, by this mechanism, is obtained by equating the hydrostatic pressure gradient to the force on the electrons $\nabla(\Sigma nkT) = -(n_e e^2/2m\omega^2)\nabla(E_{av}^2)$. Calculation gives 6 MW as the critical power for $kT = 1$ eV, with the response time being the acoustic wave transit time across the filament of 1 ns. Defining n_2 from $n_2 E_{max}^2 = 8 \times 10^{-3}$ gives $n_2 = 2 \times 10^{-13}$ esu and the self trapping length for 4 times the threshold power is 2·5 mm.

The electron density required for self focusing is inversely proportional to the beam diameter and thus the process could begin in densities of $n_e = 1{\cdot}6 \times 10^{18}$ cm^{-3} for 100 μm beam diameter with the final collapse to a filament of less than 10 μm in a region of $n_e > 2 \times 10^{19}$ cm^{-3}.

Such electron density could be formed during the cascade breakdown but might also be produced after breakdown by photoionization ahead of the plasma front. The volume rate of photoionization due to a 50 μm sphere of argon plasma assuming $T_e = 20$ eV and a three component mixture with $n^{7+} = n^{8+}$ and $n_e = 2 \times 10^{20}$ (Wheeler 1963) gives an estimate consistent with the experimental plasma conditions. Recombination continua from $n^{8+} + e \rightleftharpoons n^{7+}$ and $n^{7+} + e \rightleftharpoons n^{6+}$ together with free free transitions were calculated and the results were $1{\cdot}7 \times 10^9$, $0{\cdot}6 \times 10^9$ and $3{\cdot}4 \times 10^9$ photoionizing photons/ns sr, for the three processes, with absorption lengths in 760 torr argon of 0·03 cm, 0·033 cm and 0·0012 cm respectively (Samson 1963), giving volume ionization rates of $1{\cdot}3 \times 10^{13}$, $5{\cdot}9 \times 10^{12}$ and $2{\cdot}4 \times 10^{16}$/ns cm^3 respectively. These rates are insufficient to produce densities of the order of 10^{19} cm^{-3}, during the laser pulse, and therefore photoionization cannot play a significant role in the self focusing mechanism. Thus any mechanism involving ionization would be dependent upon direct ionization by the laser beam. This is consistent with our experimental observation that self trapping and breakdown are simultaneous to within a fraction of a nanosecond.

Heating by the laser beam in the processes discussed above will cause destruction of the filament consistent with our experimental observations. For example, for the free electron mechanism, if the filament power is 6 MW in a plasma formed from 1 atm argon with typically $n_e = 1{\cdot}6 \times 10^{19}$ and $T_e = 1$ eV, the absorption length (140 μm) in the plasma is less than the self focusing length (2·5 mm) and the rate of heating is $1{\cdot}5 \times 10^4$ eV ns^{-1}/particle. This suggests that self focusing to a 10 μm filament in such a plasma might be prevented by heating. However the excited state mechanism involves a weakly absorbing condition of the gas and therefore heating would not be significant prior to the formation of the filament though gas breakdown would occur afterwards.

In conclusion it appears that the excited state mechanism could operate in the several millimetres long focal region of the beam used in this work and that differences in the discontinuity of breakdown seen in different gases could be associated with differences in excited state resonances and the associated self focusing. Further work is in progress to investigate this phenomenon in more detail.

We are grateful to the following bodies for supporting this work: Science Research Council; UKAEA Culham; Northern Ireland Ministry of Education; to Professor D. J. Bradley for provision of research facilities and to Dr G. H. C. New for valuable discussions.

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Configuration-space three-body scattering theory

Abstract. Results are quoted for the 'physical' three-body transition operator yielding the volume-independent three-body reaction coefficient, in terms of which one computes the three-body elastic scattering rate when three initially free independently moving particles collide under the influence of short-range forces.

Consider the scattering of three particles, $\alpha = 1, 2, 3$, which for the purposes of this work may be considered elementary, spinless and distinguishable. A major objective of the theory is to determine the physical three-body reaction coefficient

$$\bar{w}(\mathrm{i} \to \mathrm{f}) \equiv \bar{w}(\boldsymbol{k}_\mathrm{i} \to \boldsymbol{k}_\mathrm{f}) \equiv \bar{w}(\boldsymbol{k}_{1\mathrm{i}}, \boldsymbol{k}_{2\mathrm{i}}, \boldsymbol{k}_{3\mathrm{i}} \to \boldsymbol{k}_{1\mathrm{f}}, \boldsymbol{k}_{2\mathrm{f}}, \boldsymbol{k}_{3\mathrm{f}})$$

expressing the probability of three-body elastic scattering in the laboratory system, from initial momenta $\hbar\boldsymbol{k}_{\alpha\mathrm{i}} = m_\alpha \boldsymbol{v}_{\alpha\mathrm{i}}$ to final momenta $\hbar\boldsymbol{k}_{\alpha\mathrm{f}}$. The reaction coefficient $\bar{w}$ is related to observation by

$$\hat{w}(\boldsymbol{k}_\mathrm{i} \to \boldsymbol{k}_\mathrm{f}) = N_1 N_2 N_3 \tau \bar{w}(\boldsymbol{k}_\mathrm{i} \to \boldsymbol{k}_\mathrm{f})$$

where $\hat{w}\,\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}\,\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}$ is the observed number of scatterings per unit time into wave-number ranges $\mathrm{d}\boldsymbol{k}_{1\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{2\mathrm{f}}$, $\mathrm{d}\boldsymbol{k}_{3\mathrm{f}}$ in a (large) volume τ containing N_α particles α per unit volume moving with the precise velocities $\boldsymbol{v}_\alpha$. Presumably $\hat{w}/\tau$ should be independent of τ, that is presumably in a correctly formulated theory the computed reaction coefficient $\bar{w}$ will be independent of τ.

If only by analogy with known results (Messiah 1962, Gerjuoy 1958) for collisions between two incident bodies one expects that

$$\bar{w}(\boldsymbol{k}_\mathrm{i} \to \boldsymbol{k}_\mathrm{f}) = \hbar^{-1}(2\pi)^{-5} |\boldsymbol{T}^\mathrm{t}(\boldsymbol{k}_\mathrm{i} \to \boldsymbol{k}_\mathrm{f})|^2 \delta(E_\mathrm{f} - E_\mathrm{i}) \delta(\boldsymbol{K}_\mathrm{f} - \boldsymbol{K}_\mathrm{f}) \qquad (1)$$

where E and $\hbar\boldsymbol{K}$ are respectively the total energy and momentum in the laboratory

system, and where

$$\bar{T}^{t}(\boldsymbol{k}_i \to \boldsymbol{k}_f) \equiv \langle f|\bar{T}^{t}|i\rangle = \bar{\psi}_f^* \bar{T}^{t} \bar{\psi}_i$$

is the centre-of-mass system matrix element of the 'physical' three-particle transition operator $\bar{T}^{t}$ between initial and final plane wave states $\bar{\psi}$. A determinative definition of T^{t}† is not immediately apparent. What is apparent is that (granting the validity of equation (1)) the physical transition operator T^{t} must differ from the customarily employed 'total' transition operator

$$T(E) = V - V\{G^{(+)}(E)\}V$$

where V is the total interaction and $G^{(+)}$ is the outgoing total Green function. The centre-of-mass system matrix elements

$$\langle f|\bar{T}|i\rangle = \bar{\psi}_f^* \bar{T} \bar{\psi}_i \tag{2}$$

contain δ-functions (Weinberg 1964, Watson and Nuttall 1967) in addition to those already appearing in equation (1) which—when directly inserted into (1)—make the right-hand side of (1) proportional to the squares of δ-functions, that is make equation (1) mathematically meaningless. Re-interpretation of the squared δ-functions along lines (Gerjuoy 1958) which yield sensible results for reaction coefficients in two-body collisions, for example

$$\{\delta(\boldsymbol{K}_f - \boldsymbol{K}_i)\}^2 = (2\pi)^{-3}\delta(\boldsymbol{K}_f - \boldsymbol{K}_i) \int d\boldsymbol{R} \exp\{i(\boldsymbol{K}_i - \boldsymbol{K}_f) \cdot \boldsymbol{R}\}$$

$$= (2\pi)^{-3}\delta(\boldsymbol{K}_f - \boldsymbol{K}_i) \int d\boldsymbol{R} \simeq (2\pi)^{-3}\tau\delta(\boldsymbol{K}_f - \boldsymbol{K}_i) \tag{3}$$

would lead to a three-body $\bar{w}$ depending on the volume τ, that is to an inconsistency with the presumption that the number of three-body scattering events in τ should be strictly proportional to τ in the limit $\tau \to \infty$. Thus the centre-of-mass matrix elements $\langle f|\bar{T}^{t}|i\rangle$ must not contain the δ-functions present in equation (2).

The foregoing assertions have motivated me to seek a configuration-space derivation of equation (1) and of a closed form expression for T^{t}. Some of the results‡ of this quest are quoted below, without proof.§ A configuration-space approach has been adopted because: (i) derivations of equation (1) in the literature (Lippmann and Schwinger 1950, Gell-Mann and Goldberger 1953, Brenig and Haag 1963) do not distinguish between T and T^{t}, and customarily are couched essentially *ab initio* in the momentum representation (which also happens to be the most natural representation for utilization of diagrammatic methods); (ii) previous investigations (Gerjuoy 1958) have shown that formulating scattering theory in configuration space can be both useful and instructive. In their totality the configuration-space results obtained do furnish a welcome confirmation of the general correctness of the customary momentum-space procedures, which usually attain their goals (e.g., a derivation of equation (1)) much more rapidly than do configuration-space procedures. Of course, this confirmation would be gratuitous were it not for the facts that the configuration-space and momentum-space formulations each involve some questionable mathematical

†Barred and unbarred symbols regularly will denote corresponding quantities in the centre-of-mass and laboratory systems respectively.

‡ Early results have been reported by Gerjuoy (1969).

§ The detailed analysis leading to these results is much too long to be reproduced here, and will have to be published elsewhere.

manipulations, after starting from equally questionable and by no means obviously identical physical assumptions. In essence, the work on three–three elastic scattering reported here can be considered to be a first step in the direction of deducing correct formal expressions for three–three reactions between composite systems; in the field of chemistry such reactions are important and often measurable.

Let

$$\Psi_i^{(+)}(E) = \psi_i(E) + \Phi_i^{(+)}(E) \tag{4}$$

be the properly and uniquely specified (e.g., via the Faddeev equations (Faddeev 1961)) solution to Schrödinger's equation describing the collision between particles 1, 2, 3 in the initial plane wave state

$$\psi_i(E) = \exp\{i(\boldsymbol{k}_{1i} \cdot \boldsymbol{r}_1 + \boldsymbol{k}_{2i} \cdot \boldsymbol{r}_2 + \boldsymbol{k}_{3i} \cdot \boldsymbol{r}_3)\} \equiv \exp(i\boldsymbol{k}_i \cdot \boldsymbol{r})$$

where, for simplicity, it is supposed that all forces are short range. Define $\bar{\Phi}_i^{t(+)}(\boldsymbol{r}; E)$ to be that part of $\bar{\Phi}_i^{(+)}(\boldsymbol{r}; E)$ which behaves asymptotically like the centre-of-mass system free space Green function

$$\bar{G}_F^{(+)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3; \boldsymbol{r}_1', \boldsymbol{r}_2', \boldsymbol{r}_3'; E) \equiv \bar{G}_F^{(+)}(\boldsymbol{r}; \boldsymbol{r}'; E)$$

when $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$ each approach infinity in such a fashion that no $\boldsymbol{r}_{\alpha\beta} = \boldsymbol{r}_\alpha - \boldsymbol{r}_\beta$ remains finite. Then I assume that the physical three-body elastic scattering is described by $\bar{\Phi}_i^{t(+)}(E)$. Now, computing the contribution made by $\bar{\Phi}_i^{t(+)}$ to the centre-of-mass system outgoing probability current (which determines the reaction coefficient in the time-independent configuration-space formulation of scattering theory) one finds equation (3) holds, with $\bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ given by

$$\lim_{r \to \infty \| \nu_f} \bar{\Phi}_i^{t(+)}(\boldsymbol{r}; E) = -C_2(E) \frac{\exp(i\bar{\rho}\sqrt{E})}{\bar{\rho}^{5/2}} \bar{T}^t(\boldsymbol{k}_i \to \boldsymbol{k}_f). \tag{5}$$

In equation (5), the notation denotes that infinity is being approached parallel to a direction ν_f—in the nine-dimensional configuration space subtended by $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$—along which no $\boldsymbol{r}_{\alpha\beta}$ remains finite as every $\boldsymbol{r}_\alpha = r_\alpha \boldsymbol{n}_{\alpha f}$ approaches infinity, where $\boldsymbol{n}_{\alpha f}$ is the direction of $\boldsymbol{r}_\alpha$ in physical space; ν_f is specified by $\boldsymbol{n}_{\alpha f}$ and the limiting ratios r_α / r_β. The final momenta $\hbar \boldsymbol{k}_{\alpha f}$ are in turn specified by ν_f, lie along $\boldsymbol{n}_{\alpha f}$, and have their expected magnitudes for scattering into directions $\boldsymbol{n}_{\alpha f}$. Furthermore, $C_2(E)$ is a known constant, depending on E and the particle masses m_α, while

$$(m_1 + m_2 + m_3)\bar{\rho}^2 = 2\hbar^{-2}(m_1 m_2 r_{12}^2 + m_2 m_3 r_{23}^2 + m_3 m_1 r_{31}^2).$$

The scattered wave $\Phi_i^{(+)}$ in equation (4) can be written in the form

$$\Phi_i^{(+)} = \Phi_{12}^{(+)} + \Phi_{23}^{(+)} + \Phi_{31}^{(+)} + \Phi_{23}^{s(+)} + \Phi_{31}^{s(+)} + \Phi_{12}^{s(+)} + \Phi_i^{d(+)} \tag{6}$$

where

$$\Phi_{12}^{(+)} = -(H_{12} - E - i\epsilon)^{-1} V_{12} \psi_i(E), \text{ etc.}$$

$$\Phi_{23}^{s(+)} \equiv \Phi_{2331}^{(+)} + \Phi_{2312}^{(+)} = -(H_{23} - E - i\epsilon)^{-1} V_{23} (\Phi_{31}^{(+)} + \Phi_{12}^{(+)}), \text{ etc.} \tag{7}$$

The quantity $\Phi_{12}^{(+)}$ is the laboratory system scattered wave when particles 1, 2, 3 collide in the absence of interactions other than $V_{12}(\boldsymbol{r}_{12})$; in other words, $\Phi_{12}^{(+)}$ is that part of $\Phi_i^{(+)}$ which is associated with the bubble diagram of figure 1(*a*). The corresponding centre-of-mass system $\bar{\Phi}_{12}^{(+)}(\boldsymbol{r})$ has a plane wave factor in configuration space, denoting the fact that, during the collision represented by figure 1(*a*),

particle 3 moves with constant velocity relative to the centre-of-mass of the entire 1, 2, 3 system. Therefore, no parts of $\bar{\Phi}_{\alpha\beta}{}^{(+)}$ behave asymptotically like the everywhere outgoing $\bar{G}_F{}^{(+)}(\boldsymbol{r};\boldsymbol{r}';\bar{E})$ as $\boldsymbol{r}\to\infty\|\boldsymbol{\nu}_f$, i.e., no parts of $\bar{\Phi}_{\alpha\beta}{}^{(+)}$ should be included in $\bar{\Phi}_i^{t(+)}$.

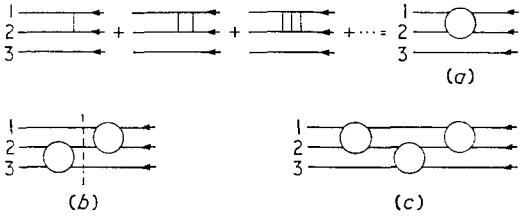

Figure 1. Scattering diagrams: (*a*) two-particle scattering between 1, 2 wherein 3 is present but non-interacting; (*b*) double scattering, first between 1, 2 and then between 2, 3; (*c*) a typical triple-scattering diagram.

The quantities $\Phi_{\alpha\beta}^{s(+)}$ in equation (6) are the parts of $\Phi_i{}^{(+)}$ associated with double-scattering bubble diagrams; for example, the $\Phi_{2312}^{(+)}$ term in equation (7) is associated with the diagram of figure 1(*b*). It can be shown that the corresponding $\bar{\Phi}_{2312}^{(+)}(\boldsymbol{r})$ contains contributions behaving like $\bar{\rho}^{-2}$ as $\boldsymbol{r}\to\infty\|\boldsymbol{\nu}_f$; therefore $\bar{\Phi}_i{}^{t(+)}$ cannot include all parts of $\bar{\Phi}_{\alpha\beta}^{s(+)}$, because $\bar{G}_F{}^{(+)}(\boldsymbol{r};\boldsymbol{r}')\sim\bar{\rho}^{-5/2}$ as $\boldsymbol{r}\to\infty\|\boldsymbol{\nu}_f$. On the other hand, $\bar{\Phi}_{2312}^{(+)}(\boldsymbol{r})$ also contains contributions behaving like $\bar{\rho}^{-5/2}$ as $\boldsymbol{r}\to\infty\|\boldsymbol{\nu}_f$, and these should be included in $\bar{\Phi}_i{}^{t(+)}$. The remaining $\Phi_i{}^{d(+)}$ contribution to $\Phi_i{}^{(+)}$ is associated with the set of all triple-order (e.g., figure 1(*c*)) and higher-order bubble diagrams. It can be seen that $\bar{\Phi}_i{}^{d(+)}(\boldsymbol{r})$ behaves asymptotically like $\bar{G}_F{}^{(+)}(\boldsymbol{r};\boldsymbol{r}')$ as $\boldsymbol{r}\to\infty\|\boldsymbol{\nu}_f$, except along an inconsequential subset $\boldsymbol{\nu}_f'$ of lower dimensionality (than the five-dimensional manifold spanned by $\boldsymbol{\nu}_f$ in the centre-of-mass system).

It now can be concluded that the physical transition amplitude $\bar{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ includes all matrix elements corresponding to triple- and higher-order bubble diagrams. In addition, $\bar{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ includes the matrix elements corresponding to the double-scattering bubble diagrams of type figure 1(*b*), if and only if each two-particle scattering fails to conserve energy, that is if and only if the intermediate state (located in figure 1(*b*) at the broken line) lies off the energy shell. In other words, the parts of $\bar{\Phi}_{2312}^{(+)}(\boldsymbol{r})$ behaving like $\bar{\rho}^{-2}$ as $\boldsymbol{r}\to\infty\|\boldsymbol{\nu}_f$ are associated with those bubble diagrams figure 1(*b*) for which the intermediate state lies on the energy shell, i.e., for which the individual bubbles in figure 1(*b*) represent actual (because they are energy-conserving) two-particle scatterings; of course, momentum always is conserved in each bubble (two-particle scattering) in figure 1(*b*). The matrix elements corresponding to the various diagrams in figure 1 are computed in accordance with the usual rules (Weinberg 1964, Watson and Nuttall 1967). In particular, the contribution of figure 1(*b*) to $\bar{T}^t(\boldsymbol{k}_i\to\boldsymbol{k}_f)$ is

$$\bar{T}_{2312}^{t}(\boldsymbol{k}_i\to\boldsymbol{k}_f)=-\frac{2\mu_{12}}{\hbar^2}\frac{\langle\boldsymbol{k}_{23f}|t_{23f}|\boldsymbol{B}\rangle\langle\boldsymbol{A}|t_{12i}|\boldsymbol{k}_{12i}\rangle}{A^2-k_{12i}{}^2} \tag{8}$$

where μ_{12} is the reduced mass of 1, 2; t_{12i} is the purely two-body transition operator for scattering of particles 1, 2 evaluated at energy $E_{12i}=\hbar^2k_{12i}{}^2/2\mu_{12}$, and similarly for t_{23f}; $\mu_{12}(\boldsymbol{v}_1-\boldsymbol{v}_2)=\hbar\boldsymbol{k}_{12}$, etc.; and $\boldsymbol{A},\boldsymbol{B}$, which denote momentum vectors in the

intermediate state, are completely specified by the given initial and final momenta $\boldsymbol{k}_i$, $\boldsymbol{k}_f$. At $A^2 = k_{12i}{}^2$, the intermediate state in figure 1(*b*) lies on the energy shell, and the right-hand side of equation (8) is replaced by zero.

If order of integration and lim $\boldsymbol{r} \to \infty \| \boldsymbol{\nu}_f$ could be interchanged in

$$(H_{23} - E - i\epsilon)^{-1} V_{23} \Phi_{12}{}^{(+)}$$

the scattered wave contribution $\bar{\Phi}_{2312}^{(+)}(\boldsymbol{r})$ would behave like $\bar{G}_F{}^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$ as $\boldsymbol{r} \to \infty \| \boldsymbol{\nu}_f$, because in this limit $\bar{G}_{23}{}^{(+)}(\boldsymbol{r}; \boldsymbol{r}') \equiv (\bar{H}_{23} - \bar{E} - i\epsilon)^{-1}$ behaves asymptotically like $\bar{G}_F{}^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$. Obviously this interchange must be unjustified, since we already know $\bar{\Phi}_{2312}^{(+)}(\boldsymbol{r})$ does not behave asymptotically like $\bar{G}_F{}^{(+)}(\boldsymbol{r}; \boldsymbol{r}')$. Nevertheless, if the interchange is performed one obtains the obvious analogue of equation (5), which analogue defines the contribution $\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ made to $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ by the $\bar{\Phi}_{2312}^{(+)}$ part of $\bar{\Phi}_i{}^{(+)}$. One finds $\bar{T}_{2312}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is precisely the usual matrix element associated with the diagram figure 1(*b*); when written in configuration space this matrix element is seen to contain a contribution proportional to $\delta(k_{12i}{}^2 - A^2)$. The same δ-function contribution is obtained if one returns to the original momentum-representation formula (8) for this matrix element—wherein $A^2 - k_{12i}{}^2 - i\epsilon$ replaces $A^2 - k_{12i}{}^2$ in the denominator—and makes the conventional re-interpretation (Brenig and Haag 1963) of

$$\lim (A^2 - k_{12i}{}^2 - i\epsilon)^{-1}$$

as $\epsilon \to 0$ when $A^2 = k_{12i}{}^2$. This one-dimensional δ-function contribution to $\bar{T}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$, if inserted into equation (1) and re-interpreted along the lines of equation (3), would yield a contribution to $\hat{w}$ proportional to $\tau^{4/3}$; a simple geometrical argument shows this is precisely the τ-dependence one expects to observe if the experimentalist measuring the three-body scattering rate does not so arrange his apparatus that actual double-scattering events are excluded. In other words, in the configuration-space approach an unwanted $\delta(k_{12i}{}^2 - A^2)$ contribution to $\bar{T}^{\mathrm{tr}}(\boldsymbol{k}_i \to \boldsymbol{k}_f)$ is obtained only because a mathematically unjustified manipulation has been performed; however, the result of this unjustified manipulation turns out to have a physically sensible interpretation. The same remarks can be made concerning other divergent expressions which arise in the configuration-space formulation of scattering theory; in general these divergences arise because of invalid mathematical operations, but lead to physically interpretable results nevertheless.

Finally one notes that the Faddeev reformulation of the Lippmann–Schwinger equation in no way mitigates the reaction rate prediction complications associated with the double-scattering diagrams figure 1(*b*). In fact, if the Faddeev equations (Faddeev 1961) are written in the form (using Faddeev's notation in essence)

$$\Phi^{(1)} = -G_{23} V_{23} \psi_i - G_F T_{23}(\Phi^{(2)} + \Phi^{(3)}), \text{ etc.}$$

then it can be seen that

$$-G_F\{T_{23}(\Phi^{(2)} + \Phi^{(3)}) + T_{31}(\Phi^{(3)} + \Phi^{(1)}) + T_{12}(\Phi^{(1)} + \Phi^{(2)})\}$$

$$= \Phi_{23}^{s(+)} + \Phi_{31}^{s(+)} + \Phi_{12}^{s(+)} + \Phi_i{}^{d(+)}.$$

This work was supported by the Advanced Research Projects Agency under Contract No. DA-31-124-ARO-D-440 and by the National Aeronautics and Space

Administration Grant No. NGR-30-011-035; the research was completed during the author's tenure as a Visiting Fellow at the Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado.

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Excitation and ionization of hydrogen by hydrogen-atom impact

Abstract. Cross sections calculated from a semi-quantal treatment are presented for the ionization of hydrogen and for the excitation of the second quantum level of hydrogen by collision with hydrogen-atoms in the ground state. Comparison with the cross sections derived from Born's approximation shows excellent agreement.

In a recent semi-quantal treatment (Flannery 1970 a) of the collision process

$$A + B(p) \rightarrow A + B(q) \tag{1}$$

at *thermal* energies, where p and q denote very highly-excited states of the target-atom B, the incoming projectile atom A is assumed to collide elastically with the atomic electron e, weakly bound to its parent ion B^+, such that the internal energy of the electron–ion pair is either increased or decreased, thereby causing excitation or de-excitation respectively. The derived cross section for (1) contained the electron–atom A elastic scattering cross section as a parameter which was taken to be isotopic, energy independent and given by its value at threshold. This procedure is valid for thermal collisions (Bates and Khare 1965). With increase to intermediate and high energies of impact, however, this choice becomes inappropriate and the correct energy-dependent (quantal) differential cross section for e–atom collisions must be used. Hence, the above treatment has been modified (Flannery 1970 b, in preparation) so as to include

the additional channels

$$A + B \rightarrow A(\Sigma) + (B^+ + e) \tag{2}$$

and

$$A + B \rightarrow A(\Sigma) + B^* \tag{3}$$

in which the projectile A, after causing ionization or excitation of the target, can remain in its initial state or be excited to all the accessible states Σ, thus giving rise respectively to elastic and inelastic contributions to the cross sections. For these neutral–neutral collisions, a binary encounter theory is still satisfactory since the interaction between A and the atomic electron is short range compared with the Coulombic interaction between the electron and its parent ion B^+. The overall description is termed semi-classical in so far as details of the electron–projectile A interaction can be furnished from a knowledge of quantum-mechanical form factors or from other similar properties, while the binary-encounter aspect of the collision is treated by classical mechanics. In this communication, we demonstrate the application of this semi-classical theory to an examination of the ionization process

$$H(1s) + H(1s) \rightarrow H(1s) + (H^+ + e) \tag{4}$$

and of the excitation of the second quantum level ($n = 2$) of hydrogen,

$$H(1s) + H(1s) \rightarrow H(1s) + H(2) \tag{5}$$

with the incident atom remaining in the ground state.

The quantal cross section for the elastic scattering by hydrogen of an electron of energy ϵ atomic units through an angle ψ is given by (Mott and Massey 1965)

$$\sigma(\epsilon, \psi) = \frac{(1 + \epsilon \sin^2 \tfrac{1}{2}\psi)^2}{(1 + 2\epsilon \sin^2 \tfrac{1}{2}\psi)^4} a_0^2 \tag{6}$$

where a_0 is the atomic unit of length and where electron exchange is neglected. By inserting (6) into equation (17) of an earlier paper (Flannery 1970 b), the integration between the angular limits $\psi^{\pm}$, introduced to yield a specified energy change, can be performed analytically to yield (instead of equation (23) of that paper)

$$\left(\frac{2\epsilon}{a_0}\right)^2 \int_{\psi^-}^{\psi^+} \frac{\sigma(\epsilon, \psi)\, \mathrm{d}(\cos\psi)}{\{(\cos\psi^+ - \cos\psi)(\cos\psi - \cos\psi^-)\}^{1/2}} = \mathscr{I}(A) - \frac{1}{\epsilon}\frac{\partial \mathscr{I}}{\partial A} + \frac{1}{6\epsilon^2}\frac{\partial^2 \mathscr{I}}{\partial A^2} \tag{7}$$

with

$$\mathscr{I}(A) = \frac{A - \tfrac{1}{2}(\cos\psi^+ + \cos\psi^-)}{\{(A - \cos\psi^+)(A - \cos\psi^-)\}^{3/2}} \pi \tag{8}$$

where A is set equal to $1 + \epsilon^{-1}$ after the differentiation is performed. For very large ϵ, (6) reduces to the Rutherford scattering formula while (7) becomes identical to the expression used for excitation by charged particles. The subsequent analysis, involving the use of (7), follows that previously outlined (Flannery 1970 b) and the excitation and ionization cross sections so derived satisfy the principle of detailed balance.

Figures 1 and 2 display the calculated ionization and the $n = 2$ excitation cross sections for (4) and (5) respectively, together with the Born results of Bates and Griffing